The application of environmental numerical simulation in pollutants migration into river basin

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Abstract：For the sustainable development of the social economy, it is very important that the water environment quality is analyzed, evaluated and predicted rationally, so that it could be planned, harnessed and managed effectively. To analyze and predict the water environment, the hydrodynamics behaviors and water pollution situations of the water body must be analyzed first based on hydrodynamics and water quality models. The objective of this work is to introduce how to establish river water dynamics and water quality model through the environment in the basin pollutant migration transformation rule, to simulate the rules and dynamics of river water pollution situation, to introduce the water quality model with geographic information system (GIS), and to apply the combination of environment numerical simulation to basin pollutant migration problem.

1. Instruction

Environment is the main living and developing condition of human being. Environmental pollution, especially the water environment pollution, has been one of the primary issues that threaten the survival of mankind. Migration motion of water as well as attenuation and transformation motion of pollutant will gradually dilute and diffuse the pollutants into the water: It's the important "self-purification of water body" [1]. However, once the pollutant level is over the self-purification, water pollution will endanger the health and life of human being.

Some laboratories have tried to adopt smaller model systems to study the migration and transformation law of pollutants under the effects of various factors, but it is rather difficult to do with the current technology. At the same time, numerical model can avoid the similarity criterion of physical model, and have the advantages of small invest and short period. This paper summarizes the theory of the pollutants' transition and translation in water body, and sums up the research progress from the numerical simulation angle and its application prospect combined with GIS, which provide an important theoretical significance and engineering practical value for water pollution research.

2. Summary of environment numerical simulation

It is of great significance for numerical simulation of environment to analyze, evaluate and predict the river water quality. Moreover, it is also of great importance to apply the diffusion rules of pollutants in water to establish the numerical model, to predict the long time influence pollutants exert on water and development tendency, and finally to take measures to control and prevent the pollutants.

In general, there are two water environment simulations. One is a physical model, which, according to the principle of similitude, simulates the fluid motion or changes of pollutants. The other is a numerical simulation, which, according to hydromechanics and migration and transformation law of pollutants, establishes numerical model to analyze the fluid motion and changes of pollutants in a certain boundary conditions and initial conditions [2].

Theoretical analysis, experimental analysis and numerical simulation are three basic approaches in the study of river hydraulic dynamics. But because of the complexity of river water environment, it will require a lot more manpower and material resources in some hydraulic model tests such as field or flume, while the similarity between physical model and real natural water environment cannot be guaranteed. Therefore, under the most conditions, numerical simulation becomes economical and practical research techniques.

According to assumption and simplification, we can establish mechanical model to find the math expression to equivalent models and create a set of mathematical equations, and finally form a mathematical model with a fixed solution,combined with initial conditions and boundary conditions. Thus, within the margin of error, adopting numerical algebra, numerical approximation, numerical differentiation and integration, ordinary differential equation and partial differential equation can lead to numerical solutions conforming to engineering application. These solutions can not only be numerical points, but also array or matrix form [3].

Nowadays, river water environment model does not just to contain diffusion in spatial and temporal distribution which can calculate several contamination index. With the rapid development in computer technique and the maturity of various theories in environment hydraulics, the discharge of pollutants and its dilution and dispersion mechanism into water can be studied. For example, radiant flux theory near zone and diffusion theory of water quality far zone, and the studies and applications of contemporary control theory, systematics and inverse problem theory all have been developed in environment hydraulics. These strike the traditional hydraulics violently, and urge water environment model nowadays to develop in the direction of integration, complication and globalization.

3. Motion characteristics of pollutants in water

The purification process of pollutants in water usually includes physical, chemical and biological process. The most fundamental process is mixing and transporting, of which temporal mean flow transport pollutants and turbulent fluctuation diffuses pollutants. Besides, attenuation and conversion further reduce pollutants concentration [4]. The chemical and biological processes decide the final destination of pollutants. These processes are influenced by temporal mean flow, turbulent fluctuation, hydrology-weather condition, chemical, biological actions and more, which makes the migration and transformation rule of pollutants in water more difficult to investigate [5].

According to the characteristics of water in nature, different types of diffusion can be classified, such as river, estuary, lake, and bay. Here, the type of diffusion in river will be introduced.

(1) flow and migration

Flow and migration generate flow action. It can only change the site of pollutants in water, but not the concentration. Under the flow and migration, transformation flux of pollutants can be calculated as follows:

$$f_x=u_x c, f_y=u_y c, f_z=u_z c \tag{1-1}$$

where, f_x, f_y and f_z represent the transformation flux in x, y and z direction, respectively; u_x, u_y and u_z represent the water velocity in x, y and z direction; c represents the concentration of pollutants in water.

(2) dispersion effect

Dispersion effect of pollutants in water includes molecular diffusion, turbulent diffusion and dispersion.

When deciding the dispersion effect of pollutants, it is important to assume that dynamic characteristics between pollutants particles and water are in agreement. The assumption satisfies the majority of dissolved pollutants in colloidal state. Molecular diffusion generates the random vibration

of molecules. Molecular diffusion meets the Fick's first law [6,7], namely that mass flux is in direct proportion to the concentration gradient of diffusate. That is,

$$I'_x = -E_M \frac{\partial c}{\partial x}, I'_y = -E_M \frac{\partial c}{\partial y}, I'_z = -E_M \frac{\partial c}{\partial z} \tag{1-2}$$

Where E_M and c represent molecular diffusivity coefficient and pollutant concentration transferred through molecular diffusion, respectively.

Molecular diffusion is an isotropy, so the negative sign above represents migration of particles pointing to the negative gradient direction. Turbulent diffusion is a dispersion phenomenon where the instantaneous value of particles in various states fluctuates randomly relative to its mean value in the turbulent flow-field in water. When the instantaneous fluctuating velocity of particles in water becomes a steady random variable, turbulent diffusion rule can be expressed with the Fick's first law, namely,

$$I^2_x = -E_x \frac{\bar{c}}{x}, I^2_y = -E_y \frac{\bar{c}}{y}, I^2_x = -E_z \frac{\bar{c}}{z} \tag{1-3}$$

Where E_x, E_y and E_z represent turbulent diffusivity in x, y and z direction.

Turbulent diffusivity follows the anisotropy due to the characteristics of turbulent flow. Turbulent diffusivity generates the calculation of time mean value. There won't be turbulent diffusion term with instantaneous value.

Dispersion arises from heterogeneous velocity distribution in the section cross, so when describing the practical movement using mean velocity at section cross, an additional action arising from heterogeneous velocity, namely dispersion, must be considered. Mass flux generated by dispersion effect can also be described with the Fick's first law:

$$I^3_x = -D_x \frac{\partial \bar{c}}{\partial x}, I^3_y = -D_y \frac{\overline{\partial \bar{c}}}{\partial y}, I^3_x = -D_z \frac{\partial \bar{c}}{\partial z} \tag{1-4}$$

Where D_x, D_y and D_z represent the dispersion coefficient in x, y and z direction.

Given that it is usual to use time mean value in practical calculation in turbulent flow, a turbulent diffusivity must be introduced. In general, molecular diffusivity value is between 10^{-5}-10^{-4}m^2/s, so turbulent diffusivity value is larger. In river, its order is 10^{-2}-10^0m^2/s. Dispersion effect usually starts when time means value spatial mean value is used, so the effect always appears in river. In general, the value of dispersion effect in river is 10^1-10^4m^2/s.

In fact, the molecular diffusion is caused by the random motion. Rivers, atmospheric problems always can be ignored on the study of the actual molecular diffusion. This is because in the flow field, the effect scale of molecular diffusion is very small, compared with turbulent diffusion or diffuses diffusion effect. But you should consider molecular diffusion when it refers to the problem of lakes and reservoirs, because in the static water environment, the molecular diffusion may become major diffusion effect.

Turbulent diffusion is caused by the random fluctation of the various states of instantaneous value relative to its time average value of turbulent flow field in the molecules. So when the medium is in the flow field with a range of velocity, if the time average value is used to describe the various states of particles, it should introduce the turbulent diffusion, and it also should consider turbulent diffusion about the study of deep sea pollution emissions, air quality simulation and the pollutant diffusion of some   rivers.

Dispersion effect is caused by uneven cross-sectional flow velocity .So the dispersion effect must be considered when it is described by using cross-sectional average flow velocity.

(3) attenuation and transformation of pollutants

Pollutants into water can be divided into two groups: conservative and non-conservative substances.

In water environment, conservative substance continuously changes its spatial position with the water flow movement. At the same time, it instantly diffuses around and decreases in concentration without changes in its total quantity due to the dispersion effect. As for non-conservative substance, its

position changes with water flow and its concentration decreases with dispersion effect in water. Besides, the concentration will also decrease quickly with the attenuation of pollutant itself.

Both experimental and practical data prove that the attenuation of pollutant in water basically conforms to the first order reaction kinetics, namely,

$$\frac{dc}{dt} = -K_c \tag{1-5}$$

Where c, t and K represent concentration of pollutant, reaction time and rate constant.

Flow and migration of river water and diffusion and attenuation of pollutant can be described using Fig 1-1.Assuming x is at x_0, quantum of pollutants into water is A and presents in straight square, and all pollutants go through x_0 at Δt (Figure 1). After a time, pollutants shift to x_1, and its quantum changes to a. If only flow, then a is equal to A, and the distribution shape of pollutants at x_1 is equal to at x_0. While if containing flow and diffusion, then a is still equal to A, but the distribution of these two is different, and transit time is also longer. If flow, diffusion and attenuation all exist, then distribution shape changes, and a is smaller than A.
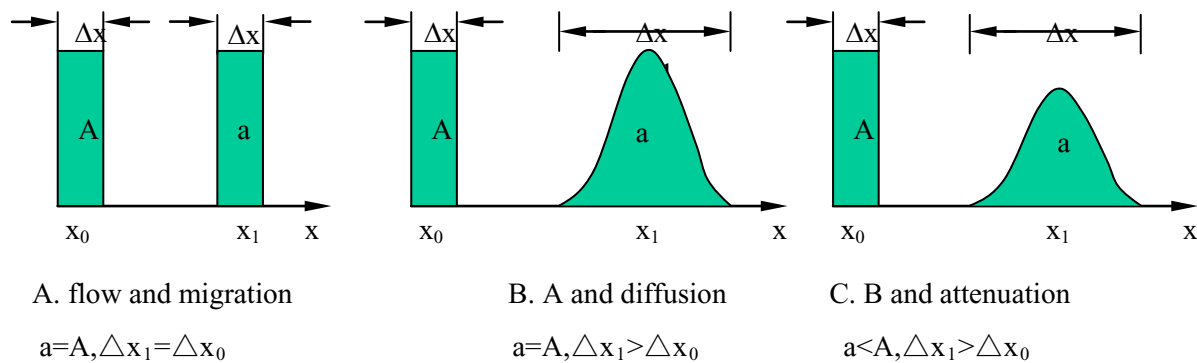

A. flow and migration	B. A and diffusion	C. B and attenuation
a=A,$\triangle x_1=\triangle x_0$	a=A,$\triangle x_1>\triangle x_0$	a<A,$\triangle x_1>\triangle x_0$

Figure 1. flow and migration, diffusion and attenuation

4. The combination of water quality model and GIS [8]

Even if standard weakly compressible SPH model has been employed for the numerical simulations [9], GIS begins to play a more and more important role in water environment numerical simulation. For GIS, it takes spatial data of geo-location as research object and spatial database as core, and uses spatial analysis and modeling method for providing multiple spatial and dynamic resource and environment information timely. It is an interpretation of geographic data characterizing geographic feature and geographic phenomenon. These data include spatial location, attributive character and time domain feature. Spatial location data describe the location of surface features, attribute data belongs to certain surface features and describe their characteristics qualitatively and quantitatively. Time domain feature is the time or moment when geographic data is collected or geographic phenomenon happens (at WPCP, such as, relevant index of source of pollution, monitoring index of fracture surface, emergency and more). Spatial location, attribute and time are three basic elements for geospatial analysis.

Because it can analyze the space features for catchment area for GIS, A. Goonetilleke[10] thinks that it has a great influence on urban hydrology, for the availability of spatial distribution database for catchment area can eliminate the attenuation of research quality due to simplification assumption. On the other hand, it also indicates the importance of accurate explanation of space-time in land use of urban catchment area. William Dixon [11] uses matrix form to combine GIS and metal forming theory to describe the structure of river network when he optimizes the sampling location of river network. Based on GIS technology and numerical simulation equation of river water environment, studying the metastatic spread rule of pollutants in water, realizing the visual representation of pollutants diffusion and discussing new method of pollution monitoring in water environment all have great practical significance in effective treatment of pollution[12]. As a kind of space, dynamic of more sources, and

multidisciplinary information science and technology GIS will be a watershed hydrological system simulation research was one of the key technologies [13].

Combined water quality model with GIS, Xia Bingxue realized the unified storage and management for mass data, made water quality simulation results more clear and visual to display and record. Meanwhile, they analyzed two-dimensional water quality into library wanzhou Yangtze river before and after the period of two-dimensional damage zone with the same method, which provided powerful technical support to relevant departments [14].

5. Conclusion and prospect

Water environment is a complex system influenced by many factors. Thus, it is unrealistic to simulate it in detail with limited time, manpower, material and financial resources, which leads to water environment model only play a role of demonstrative reference and cannot display its potential effect.

Fundamental data collection: considering that it gradually varies in the environment, it is not easy for people to observe the influence in short time. Finding the law of environment change requires tedious collection of basic data and popularization of the environmental data.

For visual research: dynamic simulation in processing of computer data shows that the research in the field needs to go deeper into the aspect of real-time control and diversification of side display.

With increasing public environmental awareness, elusion, chronicity and irreversibility of water quality have attracted more and more attention. It is a long-term and uninterrupted process for water pollutant to accumulate in the sediment of river, and it changes with the flushing of river bed. The process mechanism and its parameter selection are both very sophisticated, and the established model is still not perfect. In consequence, it's crucial for understanding the effect of pollutant in river and establishing rational equation of numerical simulation.

GIS can establish complex spatial model, manage spatial data, call water environment modules, and use computation based on water environment model and spatial data to do querying. It can be helpful to analyze spatial distribution pattern and offer decision support for river environment management. Because of parataxis of GIS and water environment model in function, even if now combined Water quality model with the GIS has a certain limitation[15], in future the combination of them may be a hot field in environment research.

Acknowledgement

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